Diffuse Reflection Boundary Conditions and Lattice Boltzmann Models for Microfluidics

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Boltzmann Equation

- Evolution equation of the one-particle distribution function $f \equiv f(\mathbf{x}, \mathbf{p})$
- BGK approximation of the collision term

$$\partial_t f + \frac{1}{m} p_\alpha \partial_\alpha f = -\frac{1}{\tau}\left[f - f^{(\mathrm{eq})}\right] \qquad \text{relaxation time } \tau = \frac{\mathrm{Kn}}{n}$$

- Hydrodynamic moments → physical quantities

particle number density: $n = \int d^3p\, f$ fluid velocity: $u_\alpha = \frac{1}{nm}\int d^3p\, f\, p_\alpha$

fluid temperature: $T = \frac{1}{3nm}\int d^3p\, f\, (\mathbf{p} - m\mathbf{u})^2$

heat flux: $q_\alpha = \frac{1}{2m^2}\int d^3p\, f\, (\mathbf{p} - m\mathbf{u})^2 (p_\alpha - m u_\alpha)$

moments of $f^{(\mathrm{eq})}$ $\mathcal{M}^{(s)}_{\{\alpha_l\}} \equiv \mathcal{M}^{(s)}_{\alpha_1\alpha_2\ldots\alpha_s} = \int d^3p\, f^{(\mathrm{eq})} \prod_{l=1}^{s} p_{\alpha_l} \quad \alpha_l \in \{1, 2, 3\}$

- Chapman-Enskog expansion + moments $\mathcal{M}^{(s)}_{\{\alpha_l\}}$ of $f^{(\mathrm{eq})}$

⇒ conservation equations ($\mathrm{Kn} \to 0$: Navier-Stokes-Fourier)

Collision terms

- Boltzmann equation with a single relaxation collision term

$$\partial_t f + \frac{1}{m} p_\alpha \partial_\alpha f = -\frac{1}{\tau}\left[f - g\right] \qquad \text{relaxation time } \tau = \frac{\text{Kn}}{n}$$

- interparticle collisions $\Rightarrow$ f is relaxing towards $g \equiv g(\mathbf{p};\{\mathcal{M}_N\})$

$g = f^{(\text{eq})}\left[\mathbf{p}; n(\mathbf{x},t), \mathbf{u}(\mathbf{x},t), T(\mathbf{x},t)\right]$ BGK collision term – extensively used

$g \equiv G(\mathbf{p};\{\mathcal{M}_N\}) f^{(\text{eq})}\left[\mathbf{p}; n(\mathbf{x},t), \mathbf{u}(\mathbf{x},t), T(\mathbf{x},t)\right]$ general case

$G(\mathbf{p};\{\mathcal{M}_N\})$ – polynomial of order N_g in $\mathbf{p}$

- particular cases:

Shakhov collision term (prescribed Prandtl number Pr) : $N_g = 3$

$$G(\mathbf{p};\{\mathcal{M}_N\}) = 1 + \frac{1-\text{Pr}}{nT^2}\left[\frac{(\mathbf{p}-m\mathbf{u})^2}{(D+2)mT} - 1\right](\mathbf{p}-m\mathbf{u})\cdot\mathbf{q} \qquad (D=3)$$

ideal gas : Pr $= 2/3$ $\qquad$ $\mathbf{q}$ = *heat flux*

BGK collision term (Prandtl number Pr $= 1$) : $G = 1$ $\qquad N_g = 0$

Gauss quadrature methods : the keystone of Lattice Boltzmann models

- LB models involve the discretization of the momentum space :

$$\mathbf{p} \mapsto \mathbf{p}_{kji} \qquad f(\mathbf{x},\mathbf{p}) \mapsto f_{kji}(\mathbf{x}) \equiv f(\mathbf{x},\mathbf{p}_{kji})$$

- Chapman-Enskog expansion: f expressed using $f^{(\mathrm{eq})}$ and $\mathcal{M}^{(s)}_{\{\alpha_l\}}$, $0 \le s \le N$

$$f(\mathbf{x},\mathbf{p}) = f^{(\mathrm{eq})} + f^{(1)} + f^{(2)} + \ldots = f^{(\mathrm{eq})} P\left[\mathbf{p}; \mathcal{M}^{(s)}_{\{\alpha_l\}}\right] \quad , \quad P \text{ - polynomial in } \mathbf{p}$$

- Recovery of the conservation equations using the Chapman-Enskog expansion requires the recovery of the hydrodynamic moments of $f^{(\mathrm{eq})}$

$$\mathcal{M}^{(s)}_{\{\alpha_l\}} = \int d^D p\, f^{(\mathrm{eq})}(\mathbf{p}) \prod_{l=1}^{s} p_{\alpha_l} \quad \mapsto \quad \widetilde{\mathcal{M}^{(s)}_{\{\alpha_l\}}} = \sum_{k,j,i} f^{(\mathrm{eq})}(\mathbf{p}_{kji}) \prod_{l=1}^{s} p_{kji\alpha_l}$$

- LB model of order $N \Leftrightarrow$ exact recovery of all moments of $f^{(\mathrm{eq})}$ up to order N

$$\boxed{\widetilde{\mathcal{M}^{(s)}_{\{\alpha_l\}}} = \mathcal{M}^{(s)}_{\{\alpha_l\}}, \qquad \forall s \le N}$$

- Equality guaranteed by Gauss quadrature methods $\Rightarrow$ vector set $\{\mathbf{p}_{kji}\}$

Cartesian coordinates in the momentum space : Gauss - Hermite Lattice Boltzmann models

- discretization of the coordinate space: $\mathbf{x} \in \mathcal{L}$ (cubic lattice in 3D)
- discretization of the momentum space

$$\mathbf{p} \mapsto \mathbf{p}_{ijk}, \qquad f(\mathbf{x}, \mathbf{p}, t) \mapsto f_{ijk}(\mathbf{x}, t) = f(\mathbf{x}, \mathbf{p}_{ijk}, t)$$

- polynomial expansion of $f^{(\mathrm{eq})}$ up to order N with respect to $\mathbf{u}$:

$$f^{(\mathrm{eq})}(\mathbf{p}; n, \mathbf{u}, T) = Q_N(\mathbf{p}; \mathbf{u}, T) f^{(\mathrm{eq})}(\mathbf{p}; n, \mathbf{u} = 0, T_{ref})$$

- the discretization procedure uses the Gauss - Hermite quadrature of order Q to achieve moments of $f^{(\mathrm{eq})}$ up to order M on the Cartesian axis

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f^{(\mathrm{eq})}(\mathbf{x},\, \mathbf{v},\, t)\, p_x^{s_1}\, p_y^{s_2}\, p_z^{s_3}\, dp_x\, dp_y\, dp_z = \sum_{i,j,k} f_{ijk}^{(\mathrm{eq})}(\mathbf{x},\, t)\, p_x^{s_1}\, p_y^{s_2}\, p_z^{s_3}$$

$$0 \le s_1,\, s_2,\, s_3 \le M \quad \Rightarrow \quad 2Q \ge N + M + 1$$

- the Cartesian components of the Q^3 vectors $\mathbf{p}_{ijk}$ $(1 \le i,\, j,\, k \le Q)$ are related to the roots of the Hermite polynomials of order Q
- $\Rightarrow$ Gauss - Hermite LB models: $HLB(N; Q_x, Q_y, Q_z)$ $\qquad Q_x = Q_y = Q_z = Q$

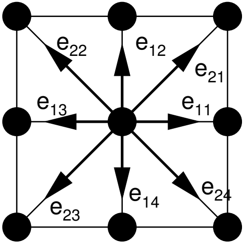
HLB models in 2D : momentum sets

$HLB(N; Q, Q, Q)$ models use the Cartesian frame in the momentum space

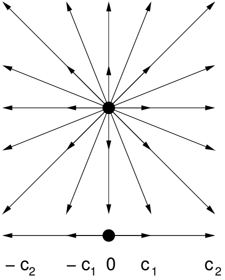
⇒ Gauss - Hermite quadrature of order Q is used on each Cartesian axis

number of vectors in the momentum set : Q^D $\qquad D \in \{1, 2, 3\}$

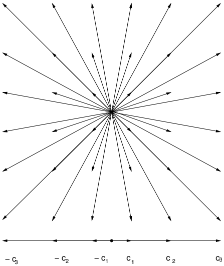
examples: $D = 2$



$Q = 3$



$Q = 5$

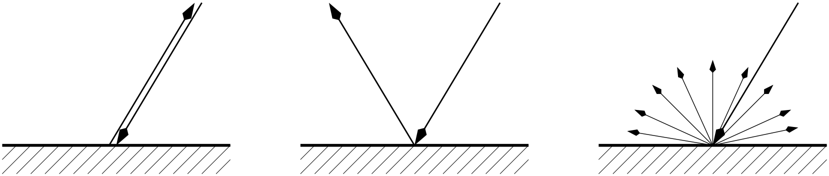


$Q = 6$

widely used since 1992 !

Boundary conditions for the distribution function

particle – wall interaction ⇒ reflected particles carry some information that belongs to the wall



bounce back | specular reflection | diffuse reflection

diffuse reflection ⇒ the distribution function of *reflected* particles is identical to the Maxwellian distribution function $\mathcal{M}(\mathbf{u}_{wall}, T_{wall})$

microfluidics ⇒ $Kn = \lambda / L$ is not negligible

⇒ velocity slip u_{slip} and temperature jump T_{jump}

Maxwell (1879): $$u_{slip} = u_{fluid} - u_{wall} = \frac{2 - \sigma_u}{\sigma_u} \, \mathrm{Kn} \, \frac{\partial u_{fluid}}{\partial n}$$

Smoluchowski (1898): $$T_{jump} = T_{fluid} - T_{wall} = \frac{2 - \sigma_T}{\sigma_T} \left[\frac{2\gamma}{\gamma + 1} \right] \frac{\mathrm{Kn}}{\mathrm{Pr}} \frac{\partial T_{fluid}}{\partial n}$$

Diffuse reflection boundary conditions

evolution equation: outgoing / incoming fluxes $\mathcal{F}^{out}_{kji\alpha}(\mathbf{x},t)$ and $\mathcal{F}^{in}_{kji\alpha}(\mathbf{x},t)$

$$f_{kji}(\mathbf{x},t+\delta t) = f_{kji}(\mathbf{x},t) - \sum_{\alpha} \frac{p_{kji\alpha}}{m}\frac{\delta t}{\delta s}\left[\mathcal{F}^{out}_{kji\alpha}(\mathbf{x},t) - \mathcal{F}^{in}_{kji\alpha}(\mathbf{x},t)\right]$$
$$-\frac{\delta t}{\tau}\left\{f_{kji}(\mathbf{x},t) - f^{(\mathrm{eq})}_{kji}(\mathbf{x},t)\Big[1 + S_{kji}(\mathbf{x},t)\Big]\right\}$$

incoming flux on the boundary:

$$\mathcal{F}^{in}_{kji\alpha}(\mathbf{x}_b,t) = -f^{(eq)}(n_w,u_w,T_w)p_{kji\alpha} = -n_w F_k(T_w)E_{kji}(\mathbf{u}_w,T_w)p_{kji\alpha}$$

with n_w computed using half-space integrals

$$n_w = \frac{\displaystyle\int_{\mathbf{p}\cdot\chi>0} f(\mathbf{x}_w,t)\mathbf{p}\cdot\chi\, d^D p}{(\beta_w/\pi)^{D/2}\displaystyle\int_{\mathbf{p}\cdot\chi<0} e^{-\beta_w(\mathbf{p}-m\mathbf{u}_w)^2}\mathbf{p}\cdot\chi\, d^D p} = -\frac{\displaystyle\sum_{p_{kji\alpha}>0}\mathcal{F}^{out}_{kji\alpha}(\mathbf{x}_b,t)}{\displaystyle\sum_{p_{kji\alpha}<0} F_k(T_w)E_{kji}(\mathbf{u}_w,T_w)p_{kji\alpha}}$$

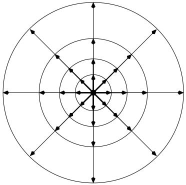
Ansumali and Karlin, Physical Review E **66** (2002) 026311; Meng and Zhang, Physical Review E **83** (2011) 036704

Spherical coordinates in the momentum space

objective: design of thermal LB models that use the spherical (3D) or polar (2D) coordinate system generalization of D2Q7 models in 2D, as well as of the thermal models introduced by Watari and Tsutahara

M.Watari, M.Tsutahara, Phys.Rev. E 036306 (2003)

2D – WT model : $4 \times 8 + 1 = 33$ momentum vectors
(4 shells + the null vector $\mathbf{c} = 0$)



- separation of variables in 3D : $\mathbf{p} \equiv \mathbf{p}(r, \theta, \varphi) = p\mathbf{e}(\theta, \varphi)$

$$e_1 = \sin\theta\cos\varphi \quad , \quad e_2 = \sin\theta\sin\varphi \quad , \quad e_3 = \cos\theta$$

$$\int d^3p\,\mathcal{I}(\mathbf{p}) = \int_0^\infty dp\,p^2 \int_{-1}^{1} d(\cos\theta) \int_0^{2\pi} d\varphi\,\mathcal{I}(p, \theta, \varphi)$$

- Equilibrium distribution function: $f^{(eq)}(\mathbf{p}; n, \mathbf{u}, T) = n\,F(p^2; T)\,E(\mathbf{p}; \mathbf{u}, T)$

$$F(p^2; T) = (\beta/\pi)^{D/2} e^{-\beta\mathbf{p}^2} \quad , \quad E(\mathbf{p}; \mathbf{u}, T) = e^{-\beta(m^2\mathbf{u}^2 - 2m\mathbf{p}\mathbf{u})} \qquad (\beta = 1/2mT)$$

- $F(p^2; T)$ has no angular dependence + discretization of p $\Rightarrow$ shells

$SLB(N;K,L,M)$: Spherical LB models (summary)

- $SLB(N;K,L,M)$: Spherical Lattice Boltzmann model that exactly recovers all moments of $f^{(\mathrm{eq})}$ up to order N and has $K \times L \times M$ momentum vectors
- The momentum vectors of the SLB(N;K,L,M) model are structured on K shells (spheres). On each shell there are L circles of latitude θ_j containing the tips of M uniformly distributed momentum vectors $\mathbf{p}_{kji} = (p_k, \theta_j, \varphi_i)$
- The vectors $\mathbf{p}_{kji} = (p_k, \theta_j, \varphi_i)$ are determined by the Gauss quadrature points (roots of generalized Laguerre / Legendre polynomials)

$$L_K^{1/2}(p_k^2) = 0 \qquad P_L(\cos\theta_j) = 0 \qquad \varphi_i = \phi + 2\pi(i-1)/M$$
$$k = 1, \dots, K > N \qquad j = 1, \dots, L > N \qquad i = 1, \dots, M > 2N$$

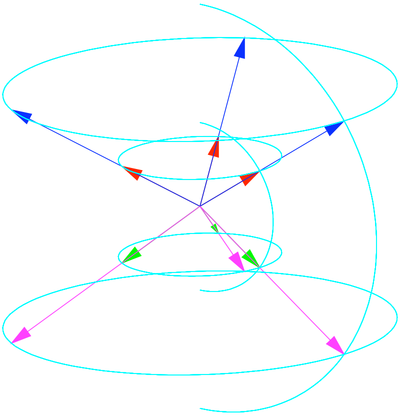
- The equilibrium distribution functions are:

$$f_{kji}^{(\mathrm{eq})} = nF_k E_{kji} \qquad F_k = \frac{\pi w_k^{(L)}}{M}\mathcal{F}(p_k^2;T) \qquad E_{kji} = w_j^{(P)} E^{(N)}(p_k, \theta_j, \varphi_i; \mathbf{u}, T)$$

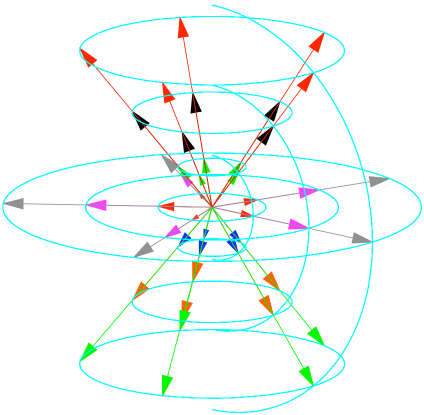
- The moments are recovered as usual in LB : $\mathcal{M}^{(s)}_{\{\alpha_l\}} = \sum_{k,j,i} f_{kji}^{(\mathrm{eq})} \prod_{l=1}^{s} p_{kji\alpha_l}$
- SLB(N;K,L,M) models have at least $(N+1)^2 \times (2N+1)$ quadrature points

more details: V. E. Ambruş and V. Sofonea, Physical Review E **86** (2012) 016708

Minimal $SLB(N;K,L,M)$ models : $SLB(N,K=N+1,L=N+1,M=2N+1)$ (1)



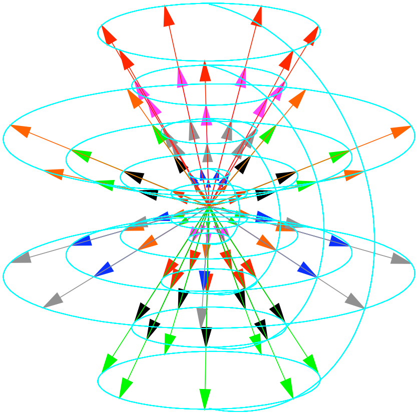
$SLB(1;2,2,3)$



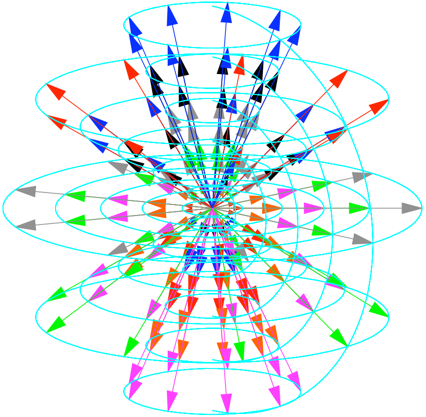
$SLB(2;3,3,5)$

V. E. Ambruş and V. Sofonea, Physical Review E **86** (2012) 016708

Minimal $SLB(N; K, L, M)$ models : $SLB(N, K = N + 1, L = N + 1, M = 2N + 1)$ (2)



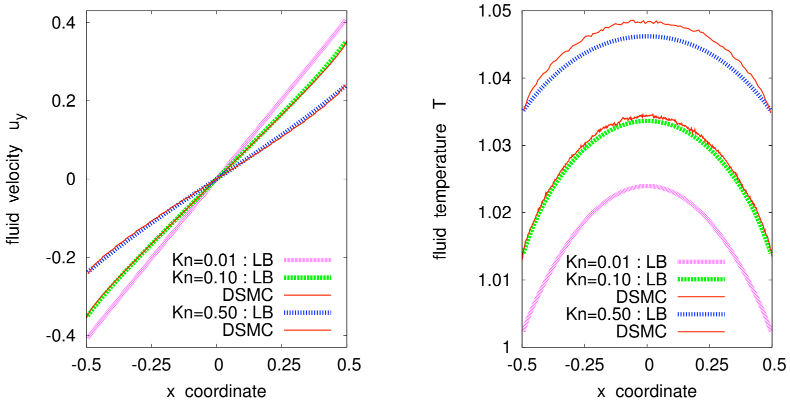
$SLB(3; 4, 4, 7)$



$SLB(4; 5, 5, 9)$

V. E. Ambruş and V. Sofonea, Physical Review E **86** (2012) 016708

Couette flow : HLB(4;10,10,10) simulation results 1/2



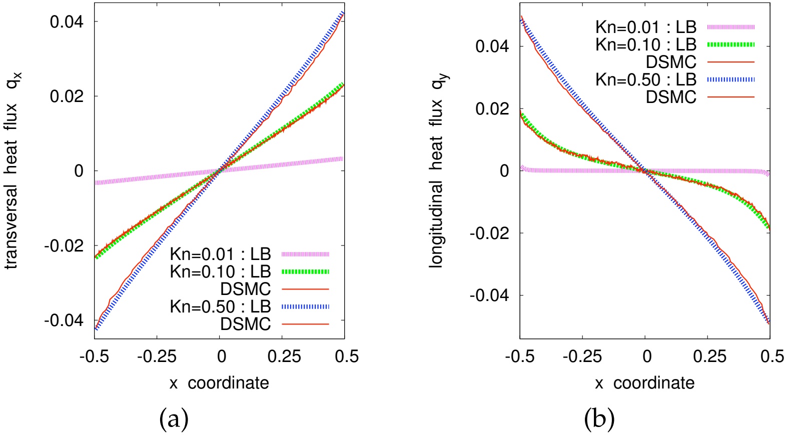
(a) (b)

Couette flow at Kn = 0.01, Kn = 0.1 and Kn = 0.5. Stationary profiles recovered with $N = 4$ and $Q = 10$: fluid velocity (a) and temperature (b).

($u_{walls} = \pm 0.42$, $T_{walls} = 1.0$, $\delta s = 1/100$, $\delta t = 10^{-4}$)

DSMC results kindly provided by Professor Henning Struchtrup (University of Victoria, Canada)

Couette flow : HLB(4;10,10,10) simulation results 2/2



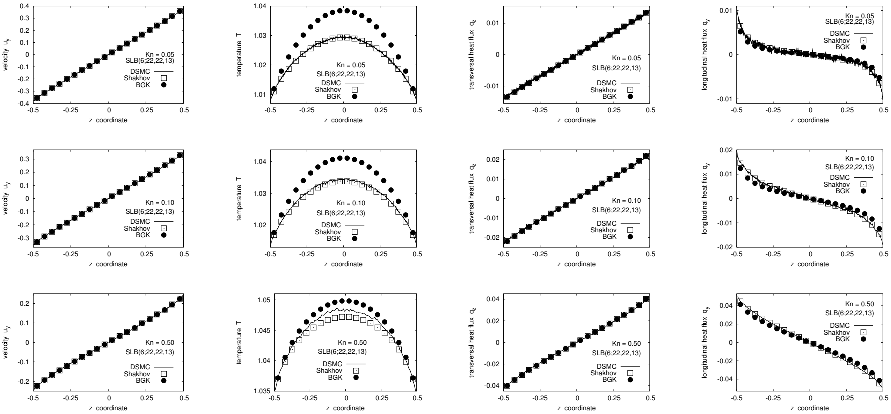
Couette flow at Kn = 0.01, Kn = 0.1 and Kn = 0.5. Stationary profiles recovered with $N = 4$ and $Q = 10$: transversal (a) and longitudinal (b) heat fluxes.
($u_{walls} = \pm 0.42$, $T_{walls} = 1.0$, $\delta s = 1/100$, $\delta t = 10^{-4}$)

DSMC results kindly provided by Professor Henning Struchtrup (University of Victoria, Canada)

Comparison BGK - Shakhov (Kn = 0.05, 0.10 and 0.50)

large *SLB* velocity sets are required to ensure good accuracy for Kn > 0.10

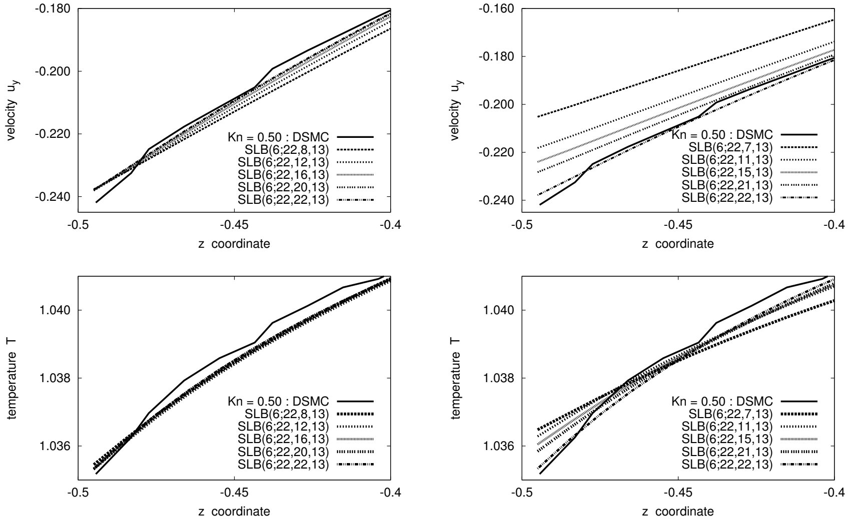
bad news : $SLB(6;22,22,13)$ is needed at Kn = 0.50 (walls $\perp z$ axis)



for Kn > 0.1 the simplified collision term (single relaxation time) is no longer appropriate !!

also observed by other authors : L.Mieussens and H.Struchtrup, Physics of Fuids **16** (2004) 2797

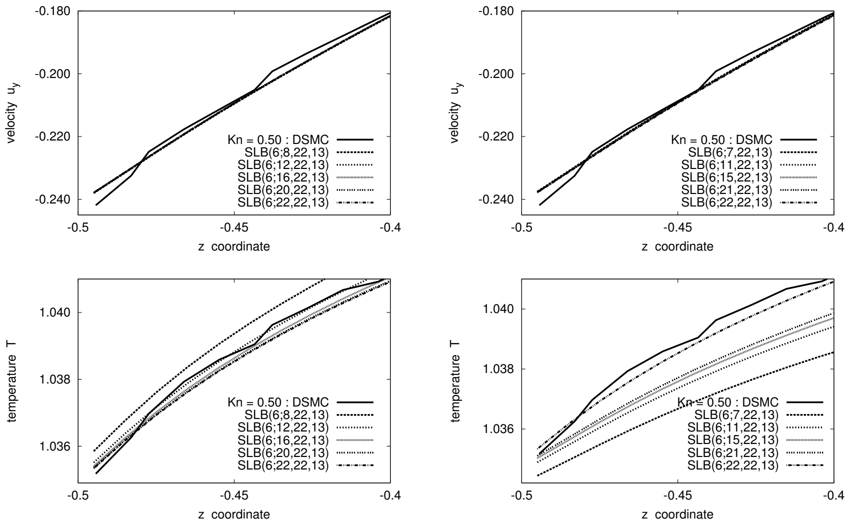
SLB(6;22,L,13) models : effect of quadrature order L



velocity and temperature profiles converge when increasing L (even or odd)

SLB models with even values of L give better results

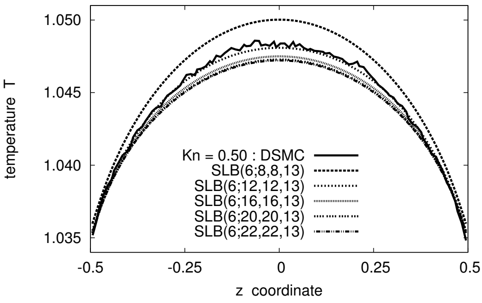
SLB(6;K,22,13) models : effect of quadrature order K

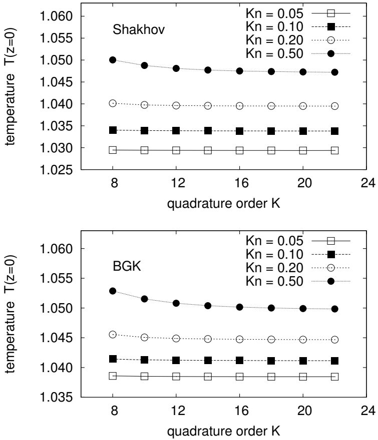


temperature profiles converge when increasing K (even or odd)

SLB models with even values of K give better results

SLB models : convergence of temperature profiles

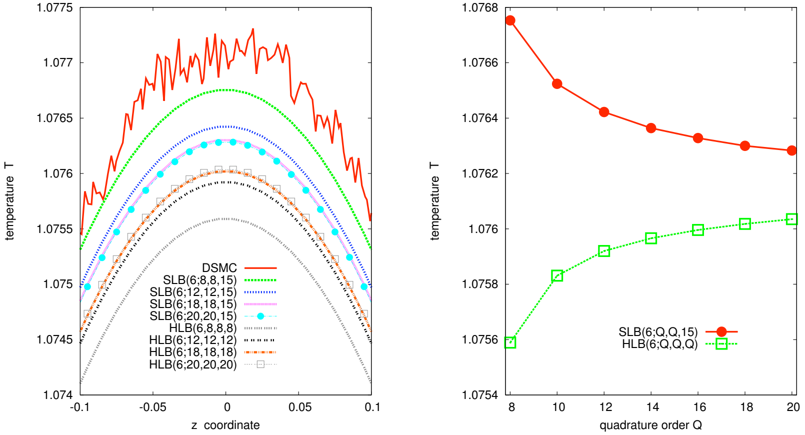




$\Rightarrow$ lower quadrature orders may be used when Kn $\rightarrow$ 0

K = L = even (z axis perpendicular to the wall)

HLB versus SLB : effect of quadrature order Q



convergence of the temperature value in the center of the channel

half space quadratures are not exactly recovered with HLB or SLB models

$\Rightarrow$ high order quadratures are needed to get accurate results for Kn $\gtrsim 0.1$

large Q$\Leftrightarrow$large velocity sets$\Leftrightarrow$computational costs + poor numerical stability

Gauss-Laguerre Lattice Boltzmann models : exact recovery of half-space integrals

- The $3D$ momentum space is split into octants:

$$\int d^3p\, P(\mathbf{p}) = \int_0^\infty dp_x \int_0^\infty dp_y \int_0^\infty dp_z \left[P(+,+,+) + P(+,+,-) + \dots\right],$$

$$P(+,-,-) \equiv P(p_x, -p_y, -p_z), \text{ etc.}$$

- $p_\alpha \in [0,\infty)$, $\alpha \in \{x,y,x\}$ $\Rightarrow$ the Gauss-Laguerre quadrature allows us to replace the integrals by sums , like in the HLB and SLB models
- unlike the HLB and SLB models, where the momentum integrals are exactly recovered over the whole space, in the Laguerre Lattice Boltzmann (LLB) models the integrals are exactly recovered over each octant $\Rightarrow$ accurate implementation of boundary conditions
- The equilibrium distribution function in LLB models is factorized as:

$$f^{(\text{eq})} = nF_xF_yF_z, \qquad F_\alpha(p_\alpha; u_\alpha, T) = \sqrt{\frac{\beta}{\pi}} \exp\left[-\beta(p_\alpha - mu_\alpha)^2\right]$$

V. E. Ambruş and V. Sofonea, to be submitted

LLB(N_x, N_y, N_z): velocity set

- Discretized momenta: roots of the Laguerre polynomials $L_{N_\alpha}(x)$:

$$p_{\alpha,k} = \begin{cases} x_{\alpha,k} & 1 \le k \le N_\alpha \\ -x_{\alpha,k-N_\alpha} & N_\alpha < k \le 2N_\alpha \end{cases} \qquad L_{N_\alpha}(x_{\alpha,k}) = 0$$

- The moments are recovered using quadrature sums:

$$\int d^3p\, f\, p_x^{n_x} p_y^{n_y} p_z^{n_z} = \sum_{i=1}^{2N_x} \sum_{j=1}^{2N_y} \sum_{k=1}^{2N_z} p_{x,i}^{n_x} p_{y,j}^{n_y} p_{z,k}^{n_z} f_{ijk}$$

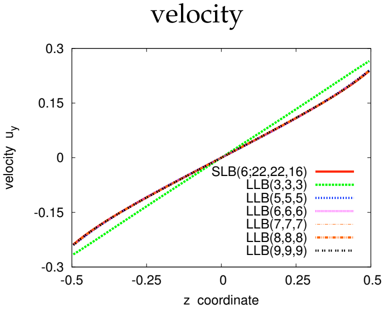
- The equilibrium distribution function can be calculated using:

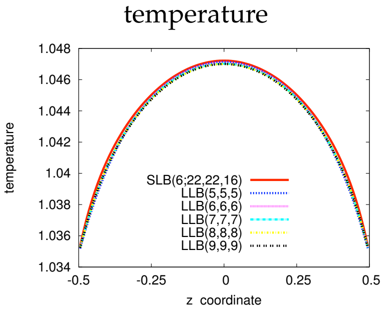
$$F_{\alpha,k} = w_{\alpha,k} \sum_{s=0}^{N_\alpha - 1} \frac{(-1)^s}{2s!} \left(\frac{mT}{2}\right)^{\frac{s}{2}} \mathcal{L}_s^{N_\alpha}(x_{\alpha,k}) \left[(1 + \text{erf} z_\alpha) P_s(z_\alpha) + \frac{2}{\sqrt{\pi}} e^{-z_\alpha^2} P_s^*(z_\alpha) \right]$$

$$w_{\alpha,k} = \frac{x_{\alpha,k}}{(N_\alpha + 1)^2 [L_{N_\alpha+1}(x_{\alpha,k})]^2} \qquad \mathcal{L}_s^{N_\alpha}(x_{\alpha,k}) = \sum_{\ell=s}^{N_\alpha-1} \binom{\ell}{s} L_\ell(x_{\alpha,k})$$

$$z_\alpha = m u_\alpha \sqrt{\beta} \qquad P_s(z) = e^{-z^2} \frac{d^s}{dz^s} e^{z^2} \qquad P_s^*(z) = \sum_{j=0}^{s-1} \binom{s}{j} \frac{d^j}{dz^j} e^{z^2} \frac{d^{s-j-1}}{dz^{s-j-1}} e^{-z^2}$$

LLB results : Couette flow at Kn=0.5 (1)



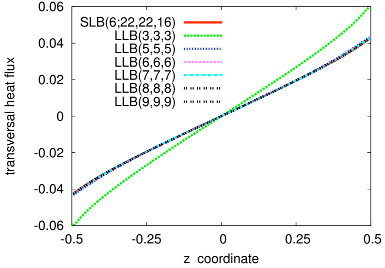


LLB(Q, Q, Q) (of order $N = Q - 1$) at Kn = 0.5

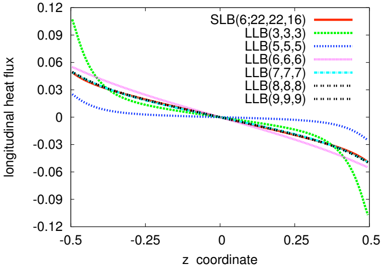
$(u_{walls} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-4})$

LLB results : Couette flow at Kn=0.5 (2)

transversal heat flux



longitudinal heat flux



model LLB(Q, Q, Q) (of order N = Q-1) has $8 \times Q^3$ momentum vectors

model SLB(N; K, L, M) (of order N) has $K \times L \times M$ momentum vectors

model HLB(N; Q, Q, Q) (of order N) has Q^3 momentum vectors

model LLB(7, 7, 7) (of order N = 6) has 2744 momentum vectors

model SLB(6; 22, 22, 12) (of order N = 6) has 6292 momentum vectors

model HLB(6; 22, 22, 22) (of order N = 6) has 10648 momentum vectors

Conclusion

- High order Lattice Boltzmann (LB) models derived by Gauss quadrature are appropriate for the investigation of micro-scale fluid flow
- LB models are able to capture microfluidic phenomena : velocity slip, temperature jump, thermal creep (transpiration), heat fluxes
- Good agreement between LB and DSMC results for Couette flow are observed up to Kn=0.5 when using the Shakhov collision term
- LB profiles (temperature, velocity, etc.) are smoother than DSMC profiles
- HLB and SLB models are not appropriate for the implementation of diffuse reflection boundary conditions because the quadratures are considered over the whole space
- LLB models are appropriate to implement the diffuse reflection boundary conditions
- Promising applications of Lattice Boltzmann models: investigation of micro-scale flow and heat transport problems in fluid systems with single or multiple components, with or without phase separation, optimization of micro-scale technological processes